Multi-Instrument Manager Tool for Data Acquisition and Merging of Optical and Electrical Mobility Size Distributions

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Abstract. Electrical mobility classification (EC) followed by Condensation Particle Counter (CPC) detection is the technique combined in Scanning Mobility Particle Sizers (SMPS) to retrieve nanoparticle size distributions in the range from 2.5 nm to 1 µm. The detectable size range of SMPS systems can be extended by the addition of an Optical Particle Sizer (OPS) that covers larger sizes from 300 nm to 10 µm. This optical sizing method reports an optical equivalent diameter, which is often different from the electrical mobility diameter measured by the standard SMPS technique. Multi-Instrument Manager (MIM™) software developed by TSI incorporates algorithms that facilitate merging SMPS data sets with data based on optical equivalent diameter to compile single, wide-range size distributions. Here we present MIM 2.0, the next-generation of the data merging tool that offers many advanced features for data merging and post-processing. MIM 2.0 allows direct data acquisition with OPS and NanoScan SMPS instruments to retrieve real-time particle size distributions from 10 nm to 10 µm, which we show in a case study at a fireplace. The merged data can be adjusted using one of the merging options, which automatically determines an overall aerosol effective refractive index. As a result an indirect and average characterization of aerosol optical and shape properties is possible. The merging tool allows several pre-settings, data averaging and adjustments, as well as the export of data sets and fitted graphs. MIM 2.0 also features several post-processing options for SMPS data and differences can be visualized in a multi-peak sample over a narrow size range.

Keywords: SMPS, OPS, NanoScan SMPS, wide-range particle measurement, data post-processing

1. Introduction

The comprehensive measurement of number concentrations and size distributions of aerosols in the sub-micrometer range has received much consideration during the past years. Assessing possible exposure to nanomaterial used in or added to products but also the investigation of airborne nanoparticles in general requires suitable and sensitive instruments. Toxicology studies reported a high rate of pulmonary deposition of nanoparticles, and also show their ability to travel from lung to systemic sites (Oberdörster et al., 2005). Additionally a high inflammation potential of nanoparticles was reported by other studies. Nanoparticles have a relative large surface area per mass which can be seen as interaction interface. Therefore it has been concluded that particles in the nanometer range are more biologically active (Gurr et al., 2005).

Measuring exposure to nanoparticles has been conducted in academic research using high-end instrumentation in the laboratory. With the need to move these measurements out of the laboratory into the field to study indoor air quality and occupational health and safety, more compact and easy to use instrumentation is required to characterize the aerosol.
Commonly the technique of choice is electrical mobility classification followed by Condensation Particle Counter (CPC) detection. Both are typically combined in a Scanning Mobility Particle Sizer (SMPS) to retrieve nanoparticle size distributions in the range from 2.5 nm to 1 µm. During the last NanoSafe Conference we introduced the NanoScan SMPS (TSI model 3910, Tritscher et al., 2012), which is a novel, portable nanoparticle sizing and counting instrument that is capable of covering the range from 10 to 420 nm. Its straightforward portability is a key to help in source identification measurements.

The detection size range of SMPS systems can be extended by the addition of an Optical Particle Sizer (OPS, TSI model 3330) that covers larger particle sizes from 300 nm to 10 µm and is also a portable and compact device. Its optical sizing method reports an optical equivalent diameter, which is often different from the electrical mobility diameter measured by the standard SMPS technique. Discrepancies between different measurement principles as well as the challenges in combining size spectral data were the motivation to develop a small but powerful data merging tool. Multi-Instrument Manager (MIM™) software was introduced by TSI to integrate algorithms that facilitate the merging of SMPS data based on electrical mobility diameter with data dependent on an optical equivalent diameter into one single, wide-range data set. Here we present the functionality of MIM 2.0, the next-generation of the data merging tool and give some data merging, data acquisition and SMPS post-processing examples.

2. Method and Instrumentation

The Multi-Instrument Manager (MIM™) software is a MATLAB-based tool that allows reviewing, averaging, merging and post-processing data from TSI SMPS spectrometers equipped with the previous 3080 and the new 3082 Electrostatic Classifier generations, NanoScan SMPS (TSI model 3910) and/or OPS (TSI model 3330) instruments. MIM software was introduced by TSI after the original development of dedicated algorithms (Han et al., 2011) that facilitate merging SMPS data based on electrical mobility diameter with data based on optical equivalent diameter to compile a single, wide-range data set. MIM 2.0 features increased channel resolution of up to 128 size channels per decade of recorded SMPS raw data files, comparison of SMPS correction steps and combination of multiple units. One of the key features when merging OPS with electrical mobility distributions is that the software takes aerosol optical properties into account by automatically determining an overall aerosol effective refractive index that was used to adjust the merged data. Thus an indirect and average characterization of aerosol optical and shape properties is possible.

In Figure 1 we show an example for measurements from SMPS and OPS with the resulting composite fit. The merging procedure is heavily dependent on the particle type, concentration and distribution.

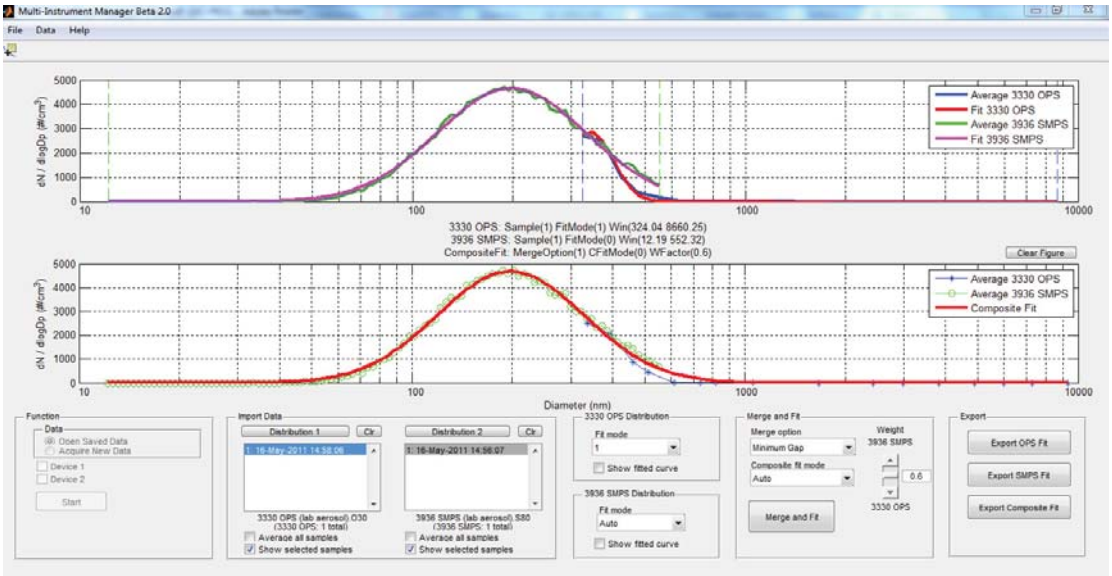

Figure 1: Size distribution of ambient air aerosol from SMPS and OPS measurement displayed in the MIM 2.0 view. The top panel shows the individual size distributions as well as their average and the lower graph shows the merged curve as a result in red.

Data merging is done is by combining two size distribution measurements that have been uploaded, which can also be the averages of several size distributions. The Merge and Fit panel (data control area, see Figure 1) allows parameterization of the merge algorithm. The merge option selection panel includes "No Correction", "Minimum Gap" and "Calibration Data". The software's "Minimum Gap" option will seek to minimize the gap (global minimum) between the SMPS and the OPS distributions by varying the real part of the refractive index and shape correction factor of the OPS data. Typical values displayed for the real part of refractive index are between 1.3 to 1.8, and for the shape correction factor 0.8 to 1.05. The optimal refractive index found by the algorithm will provide the "best fit" to the data but is not necessarily equivalent to the bulk refractive index of the aerosol of interest. However, in many cases it can help to provide further insight into the characteristics of the optical aerosol properties.

For the "Calibration Data" option, the algorithm seeks to minimize the difference between the calibration data and reference monodisperse sizes by varying the shape factor as well as the real and imaginary part of the refractive index. This option is only possible if the user created a calibration data set earlier on. As the OPS is calibrated with polystyrene latex (PSL) reference particles, the optically determined particle diameters from the OPS may differ from physical particle diameters due to material properties such as refractive index, morphology and shape. By using an Electrostatic Classifier to supply monodisperse aerosols to the OPS, the OPS can be calibrated to measure mobility diameter. Particles used for such a calibration should be the same or as a minimum comparable to the particles sampled as size distributions that should be merged.

Additional settings like fit mode selection (e.g. auto/1/2/3) help to find the best fitting curve and the weighting option allows prioritizing data either based on SMPS/NanoScan SMPS or OPS in the overlapping region. All merged size distributions and data sets as well as fitted graphs can be exported. MIM 2.0 permits several pre-settings, data averaging and adjustments. More details on the different options and settings can be found in the MIM user guide.

3 Results and Discussion

3.1. Multi-Modal Laboratory Aerosol

Data merging of uni-modal size distributions as shown in Figure 1 is typically not very challenging for any fitting procedure. Therefore a laboratory aerosol was generated from two different aerosol sources and subsequently measured. We used Arizona Road Dust in a Small Scale Powder Disperser (SSPD, TSI model 3433) and a sucrose solution in a constant output atomizer (TSI model 3076) with diffusion dryer. NanoScan SMPS and OPS were used to detect and determine the size distribution of the mixed lab aerosol. The two instruments sampled the laboratory aerosol from a mixing chamber (blue "bean pot" as shown in Figure 2).

The aerosol generation was largely stable over a time span of several minutes, which is displayed in the several thin curves in the top panel of Figure 3. The average size distributions from NanoScan SMPS and OPS were used for the data merging but the same is possible also for individual scans. Figure 3 shows the data merging result using the Minimum Gap option in the lower panel and suggested a three modal composite fit. The software tool can easily deal with multi-modal distribution as these results demonstrate.

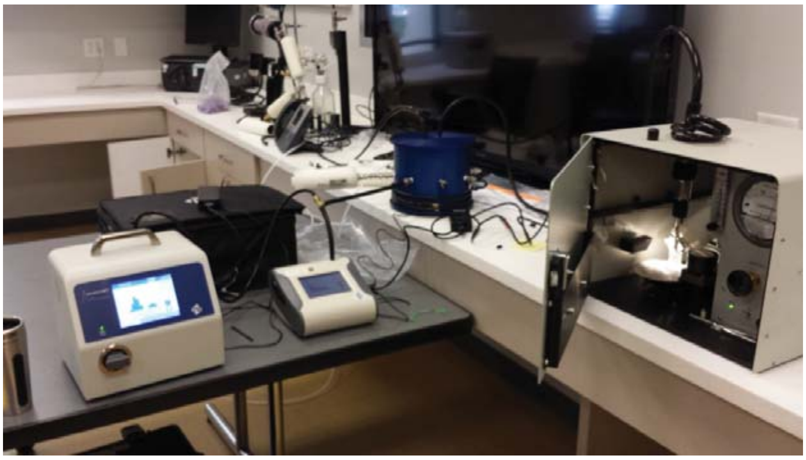

Figure 2: Setup with NanoScan SMPS and OPS for laboratory-generated bi-modal aerosols. A constant output atomizer and a Small Scale Powder Disperser (SSPD) were used for the primary generation and the aerosol was subsequently mixed inside the blue mixing manifold.

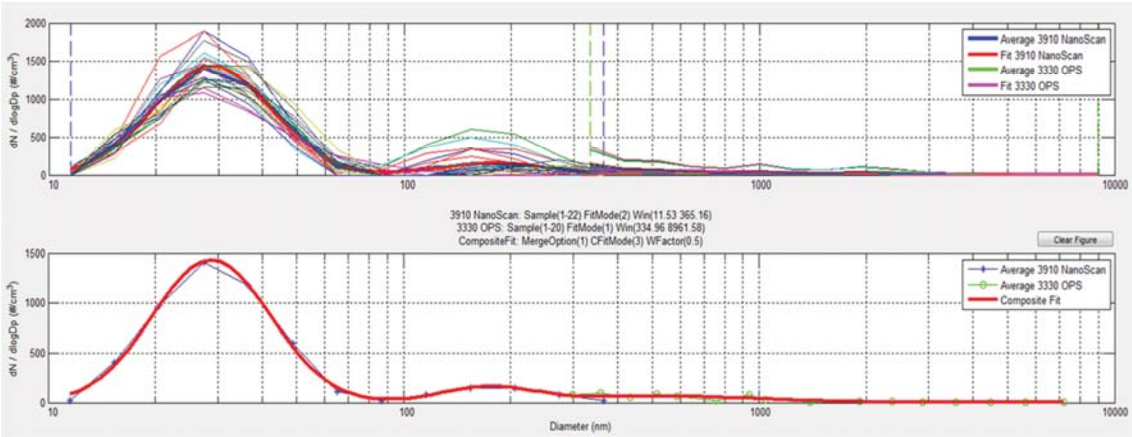

Figure 3: Multimodal size distributions of a laboratory aerosol displayed in the MIM 2.0 view. Minimum gap merging and three modal fitting were pre-selected. The red curve in the lower panel shows the resulting fit.

3.2. Case Study Fireplace

The capabilities of MIM were further tested for a real-world aerosol that requires a wide measurement size range. In a brief case study we collected data with NanoScan SMPS and OPS instruments from a wood-burning fireplace. The fireplace was located in the living room of a domestic building. The ambient air in the room where the fireplace is located was monitored for two hours, with the instruments set to 1 min sample time per run. Compressed wood was used as fuel, which was again added after one hour of fireplace operation. The details of the actual measurement setup are considered to be of secondary importance here as the main purpose of this work is not the evaluation of the burning behavior but collecting exemplary data for use with the new MIM 2.0 software.

Figure 4 summarizes the results during the two hour measurement period complemented with photos of the corresponding burning phases. The top panels show 1 min size distribution scans and their average value and the red curves in the lower panels present the merged size distribution curves, respectively. The size distribution shown ranges from 10 nm to 10 µm. A nucleation mode develops during the measurement and after an hour forms a stable mode around 20-30 nm, while the accumulation mode at around 100 nm decreases relatively and shifts slowly to size larger than 100 nm. For a more comprehensive study that describes the complete development of the bimodal size distribution of the fireplace emission, smaller average intervals should be chosen as some information gets lost, especially in the beginning when size distributions vary rapidly. However, here we focus exclusively on the MIM processing option and using average values before merging is one possible approach if not every single size distribution should be merged individually.

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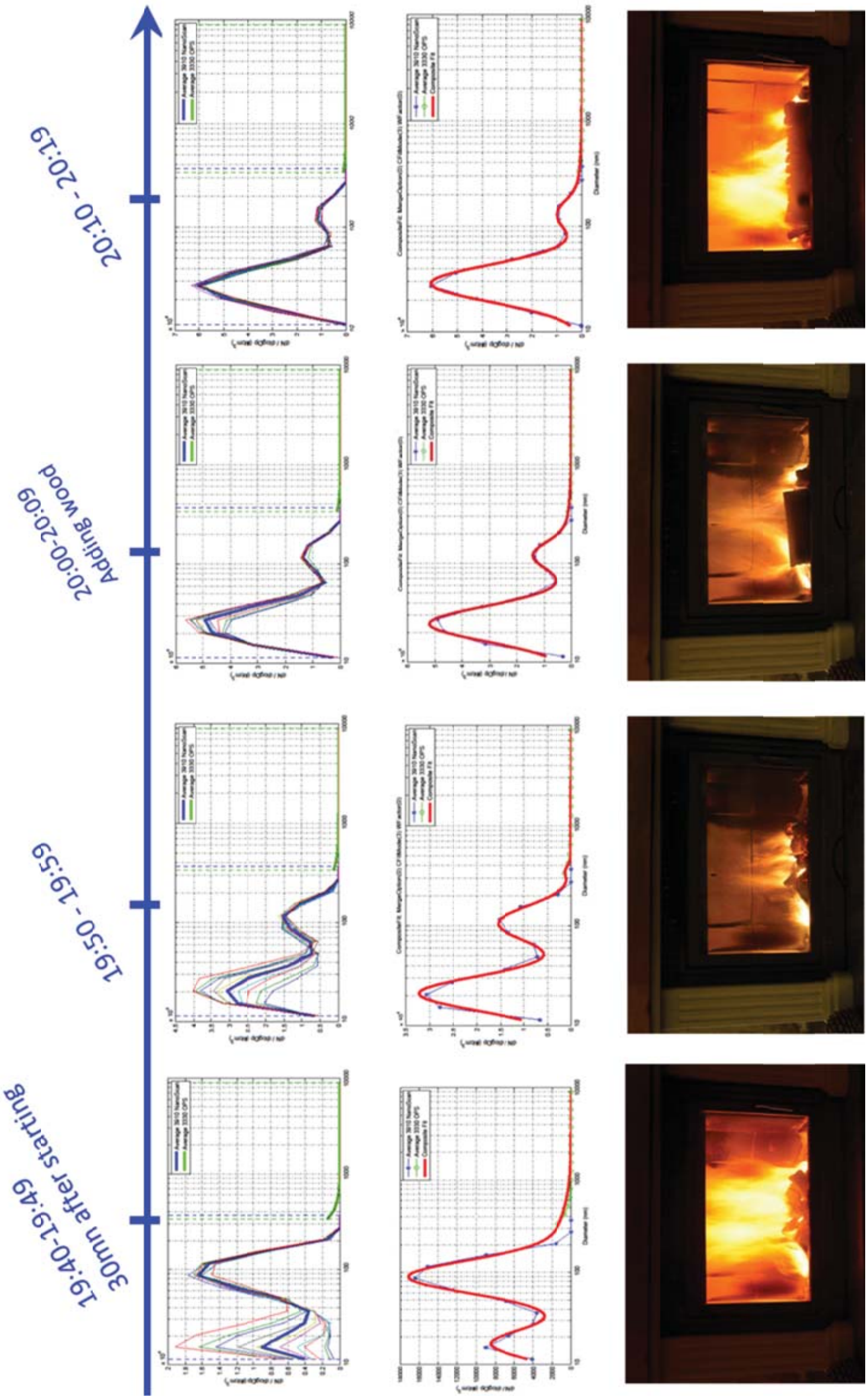

Figure 4: Development of measured aerosol size distribution during a fireplace burning cycle. The upper panels show the individual measured size distributions for NanoScan SMPS and OPS and their average (bold curve). The merging results of the bimodal size distributions are shown in the middle panel and on the bottom photographs that illustrate the corresponding burning phases.

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3.3. Post-processing of SMPS Data

Other than the actual merging of measurement data, MIM 2.0 allows also post-processing electrical mobility size distribution data recorded with the high-resolution component SMPS. Data from the recently-introduced SMPS, TSI model 3938 (Tröstl et al., 2014) that uses a newly-developed Electrostatic Classifier (TSI model 3082) as well as most data from SMPS based on the 3080 model Electrostatic Classifier can be loaded for re-processing.

There are several configuration options within the SMPS Settings window for the data inversion that is applied. The main panels for modifications are Classifier Platform, Time Delay, Correction and Channel Resolution. Three drop-down menus exist within the Classifier Platform panel to modify the data corrections for impactor size, DMA high voltage polarity and neutralizer type that were used when collecting the data. The Time Delay panel allows for adjustment of the amount of time it takes for an aerosol to travel from the outlet of the classifier DMA to the CPC detector.
Figure 5 gives an example of how the Correction panel in the SMPS Settings window of MIM can be used to apply physical property adjustments. In this example a multi-peak particle size distribution in the low diameter range sub-20 nm is shown without corrections (blue curve). The same size distribution with multiple charge and diffusion loss corrections applied can be directly compared to the uncorrected curve in the same graph. Accounting for diffusion losses results in a higher concentration, while the multi-charge correction only has a negligible effect in this example due to the small, completely single charged particle diameters (Figure 5).

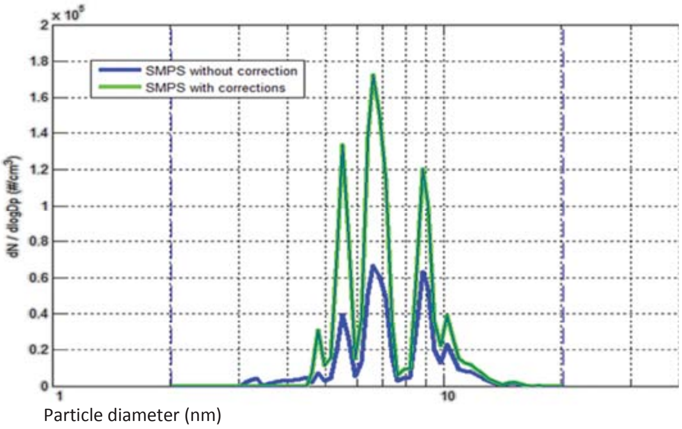

Figure 5: Direct comparison of SMPS size distribution with and without corrections for diffusion losses and multiple charging in MIM.

A second SMPS post-processing example is shown in Figure 6 for the Channel Resolution panel. The MIM software enables increasing the displayed SMPS size resolution from 64 channels per decade to 128 channels per decade by reanalyzing the raw measurement data, which are typically not accessible. Results from a multi-peak scan in the lower nanometer range displayed with 64 channels per decade and 128 channels per decade are shown in Figure 6. This higher resolution can be useful in cases like the selected example but there are many size distributions which do not necessarily benefit from an increased channel resolution. We also want to point out that it is only possible to reprocess the data for higher size resolution if the SMPS spectrometer settings during the collection of the raw data were set accordingly.

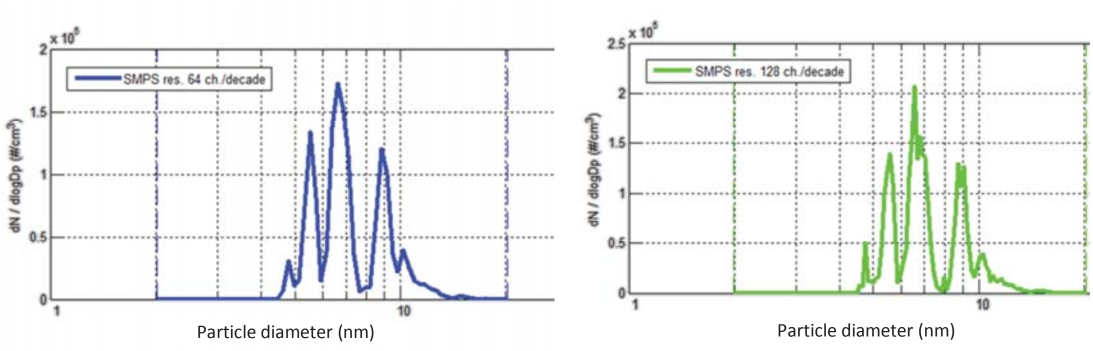

Figure 6: Multi-peak scan in the lower nanometer size range of the SMPS with different size resolution. The standard resolution is 64 channels per decade (blue). The increased resolution with 128 channels per decade (green) can be reprocessed from raw data.

4. Conclusions

In this paper we describe the new Multi-Instrument Manager (MIM 2.0) software which is an easy to use tool to merge and post-process data from commonly used TSI SMPS, NanoScan SMPS and OPS instruments. Merging of size distributions from electrical mobility and optical diameter based instruments can be done in three different ways and by selecting several fitting options with the objective of retrieving one single size distribution over a wide particle size range. Case studies for laboratory and fireplace aerosols conducted with NanoScan SMPS and OPS instruments demonstrated that curve fit distributions with up to three modes of lognormal distribution from nano- and micrometer sizing instruments can be merged well up to three modes of lognormal distribution. Also online data acquisition over a wide range as well as data processing from two instruments of the same type are now possible.

In addition we have shown that MIM is capable of doubling the size resolution of existing SMPS data to 128 channels per decade. Recorded SMPS data sets can be reprocessed to take into account different post-processing settings and the applied corrections can be displayed for direct comparison. This feature provides SMPS users better control and more options to evaluate and process size distribution data sets. While MIM software does not have the purpose to replace instrument measurement software such as the Aerosol Instrument Manager (AIM, TSI Inc.), it is an additional tool that helps to develop a better understanding of aerosol size distribution data over a wide size range.

5. References

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6. Supplementary comment

SMPS/NanoScan SMPS/OPS customers can download MIM 2.0 software free of charge from the following website: www.tsi.com/MIM .